The one-dimensional Hubbard Model and Exact Diagonalization

(Due date: 3rd of February 2014)

The one-dimensional Hubbard model is given by

\[
H = -t \sum_{i,\sigma} \left( c_{i,\sigma}^\dagger c_{i+1,\sigma} + c_{i+1,\sigma}^\dagger c_{i,\sigma} \right) + \frac{U}{2} \sum_{i,\sigma} n_{i,\sigma} n_{i,-\sigma},
\]

(1)

where \( c_{i,\sigma}^\dagger \) and \( c_{i,\sigma} \) are the creation and annihilation operators for an electron at site \( i \) with spin \( \sigma \) and \( n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma} \) is the corresponding occupation number operator. The first term in equation (1) is a kinetic hopping term which allows energy gain by delocalizing the electrons into itinerant states. These hopping processes have amplitude \( t \). The second term describes the on-site Coulomb repulsion \( U \) between electrons sharing the same orbital.

To study the model we consider the occupation number representation which includes states describing all possible distributions of \( N \) electrons over the \( L \) lattice sites of a chain of ions. In particular, we label these sites with the following convention

\[
\begin{array}{cccc}
\square & \square & \cdots & \square \\
L-1 & 2 & 1 & 0
\end{array}
\]

(2)

We can represent the up- and down-spin configurations in the computer separately by assigning to each lattice site a 1 if the site is occupied or a zero if it is not. For example, a state that has five electrons on an eight-site chain with three up spins and two down spins is represented in this notation as

\[
|00101010\rangle_\uparrow |00100100\rangle_\downarrow.
\]

(3)

The up-spin electrons are at sites 1, 3 and 5 while the down-spin electrons are at sites 2 and 5. The remaining sites are unoccupied.
ASSIGNMENT: (40 points)

1.- Find the ground-state energy of the Hubbard model on rings (chains with periodic boundary conditions) with 4, 6, 8, 10, 12 and 14 sites at half-filling, i.e. when the number of sites equals the number of electrons and there is the same number of up-spin and down-spin electrons in the system. Compare your results with the exact solution which is given by

\[ E_0(U) = -4L \int_{0}^{\infty} \frac{J_0(\omega)J_1(\omega)}{\omega \left(1 + \exp(\omega U/2)\right)} d\omega, \]

where \( J_n(\omega) \) is the Bessel function of the first kind (of order \( n \)) and \( L \) is the number of sites on the ring. The hopping amplitude is set to one.

2.- Calculate the ground-state expectation value of the operators \( n_{i,\uparrow} \pm n_{i,\downarrow} \) for different values of the interaction \( U \).

DISCUSSION: (10 points)
On the 4th of February you are expected to give a short (15min) presentation where you will:

- Introduce the problem you worked on.
- Give technical details about the numerical problem and how you dealt with it.
- Present your final results.
- Answer the questions of the audience.